Lecture 7. Terrestrial infrared radiative process. Part 1: Line-by-line approach.

Objectives:

- 1. Fundamentals of the thermal IR radiative transfer.
- 2. Line-by-line computations of radiative transfer in IR.
- 3. Spectroscopic databases.

Required reading:

L02: 4.2.2-4.2.3

1.1. Fundamentals of IR radiative transfer.

Recall the equation of radiative transfer (Eq.[2.18 a, b], Lecture 2) for upward and downward intensities in the plane-parallel atmosphere

$$\mu \frac{dI_{\lambda}^{\uparrow}(\tau;\mu;\varphi)}{d\tau} = I_{\lambda}^{\uparrow}(\tau;\mu;\varphi) - J_{\lambda}^{\uparrow}(\tau;\mu;\varphi)$$

$$-\mu \frac{dI_{\lambda}^{\downarrow}(\tau;-\mu;\varphi)}{d\tau} = I_{\lambda}^{\downarrow}(\tau;-\mu;\varphi) - J_{\lambda}^{\downarrow}(\tau;-\mu;\varphi)$$
[2.18a]

$$-\mu \frac{dI_{\lambda}^{\downarrow}(\tau;-\mu;\varphi)}{d\tau} = I_{\lambda}^{\downarrow}(\tau;-\mu;\varphi) - J_{\lambda}^{\downarrow}(\tau;-\mu;\varphi)$$
[2.18b]

and its solutions (Eq.[2.19a,b], Lecture 2):

$$I_{\lambda}^{\uparrow}(\tau;\mu;\varphi) = I_{\lambda}^{\uparrow}(\tau_1;\mu;\varphi) \exp(-\frac{\tau_1 - \tau}{\mu})$$

$$+\frac{1}{\mu} \int_{\tau}^{\tau_1} \exp(-\frac{\tau' - \tau}{\mu}) J_{\lambda}^{\uparrow}(\tau'; \mu; \varphi) d\tau'$$
 [2.19a]

$$I_{\lambda}^{\downarrow}(\tau;-\mu;\varphi) = I_{\lambda}^{\downarrow}(0;-\mu;\varphi) \exp(-\frac{\tau}{\mu})$$

$$+\frac{1}{u}\int_{0}^{\tau}\exp(-\frac{\tau-\tau'}{u})J_{\lambda}^{\downarrow}(\tau';-\mu;\varphi)d\tau'$$
 [2.19b]

<u>Infrared radiative transfer in the atmosphere:</u>

Assuming non-scattering medium in the local thermodynamical equilibrium:

the source function is given by the Plank's function $B_{\lambda}(T)$ (see Lecture 3)

and $\beta_{e,\lambda} = \beta_{a,\lambda} = k_{\lambda} \rho$, where k_{λ} is the mass absorption coefficient.

Assuming that the thermal infrared radiation from the earth's atmosphere is independent on the azimuthal angle ϕ , the equation of infrared radiative transfer for the monochromatic upward and downward intensities can be expressed in the wavenumber domain as

$$\mu \frac{dI_{v}^{\uparrow}(\tau;\mu)}{d\tau} = I_{v}^{\uparrow}(\tau;\mu) - B_{v}(T)$$

$$-\mu \frac{dI_{v}^{\downarrow}(\tau;-\mu)}{d\tau} = I_{v}^{\downarrow}(\tau;-\mu) - B_{v}(T)$$
[8.1a]

and its solutions as

$$I_{\nu}^{\uparrow}(\tau;\mu) = I_{\nu}^{\uparrow}(\tau_{1};\mu) \exp\left(-\frac{\tau_{1} - \tau}{\mu}\right) + \frac{1}{\mu} \int_{\tau}^{\tau_{1}} \exp\left(-\frac{\tau' - \tau}{\mu}\right) B_{\nu}(T(\tau')) d\tau'$$
[8.2a]

$$I_{\nu}^{\downarrow}(\tau;-\mu) = I_{\nu}^{\downarrow}(0;-\mu) \exp(-\frac{\tau}{\mu})$$

$$+ \frac{1}{\mu} \int_{0}^{\tau} \exp(-\frac{\tau - \tau'}{\mu}) B_{\nu}(T(\tau')) d\tau'$$
[8.2b]

To solve Eqs.[8.2a, b] for the whole atmosphere with total optical depth $\tau_{1}=\tau_{v}^{*}$, two boundary conditions are required:

Surface: assumed to be a blackbody in the IR emitting with the surface temperature T_s,

$$I_{\nu}^{\uparrow}(\tau_{\nu}^{*},\mu) = B_{\nu}(T_{s}) = B_{\nu}(T_{s}(\tau_{\nu}^{*})) = B_{\nu}(\tau_{\nu}^{*})$$

Top of the atmosphere (TOA), $\tau_v = 0$: no downward thermal emission

$$I_{\nu}^{\downarrow}(0,-\mu)=0$$

Using the above boundary conditions, the formal solutions for monochromatic upward and downward intensities are

$$I_{\nu}^{\uparrow}(\tau;\mu) = B_{\nu}(\tau^{*}) \exp(-\frac{\tau^{*} - \tau}{\mu}) + \frac{1}{\mu} \int_{\tau}^{\tau^{*}} \exp(-\frac{\tau' - \tau}{\mu}) B_{\nu}(\tau') d\tau'$$

$$I_{\nu}^{\downarrow}(\tau;-\mu) = \frac{1}{\mu} \int_{0}^{\tau} \exp(-\frac{\tau - \tau'}{\mu}) B_{\nu}(\tau') d\tau'$$
[8.3a]

✓ The formal solutions for monochromatic upward and downward intensities can be
also expressed in terms of monochromatic transmittance.

By definition, the monochromatic transmittance is

$$T_{\nu}(\tau;\mu) = \exp(-\frac{\tau_{\nu}}{\mu})$$

and the differential form is

$$\frac{dT_{\nu}(\tau;\mu)}{d\tau} = -\frac{1}{\mu} \exp(-\frac{\tau_{\nu}}{\mu})$$

Thus the formal solutions for monochromatic upward and downward intensities given by Eq.[8.3a,b] in terms of transmittance are:

$$I_{\nu}^{\uparrow}(\tau;\mu) = B_{\nu}(\tau^*)T_{\nu}(\tau^* - \tau;\mu)$$

$$I_{\nu}^{\uparrow}(\tau;\mu) = B_{\nu}(\tau^*)T_{\nu}(\tau^* - \tau;\mu)$$
$$-\int_{\tau}^{\tau^*} B_{\nu}(\tau') \frac{dT_{\nu}(\tau' - \tau;\mu)}{d\tau'} d\tau'$$

$$I_{\nu}^{\downarrow}(\tau;-\mu) = \int_{0}^{\tau} B_{\nu}(\tau') \frac{dT_{\nu}(\tau-\tau';\mu)}{d\tau'} d\tau'$$

1.2. Line-by-line (LBL) computations of radiative transfer in IR.

LBL method is considered to be an "exact" computation of radiative transfer in the gaseous absorbing/emitting inhomogeneous atmosphere, accounting for all (known) gas absorption lines in the wavenumber range from 0 to about 23,000 cm⁻¹.

For a given wavenumber **v**:

For the j-th atmospheric layer:(homogeneous; temperature T_j , pressure p_j , length ΔZ_j)



Absorption coefficient $k_{\nu,j,n}$ is

$$k_{v,j,n} = \sum_{l=1}^{L} k_{v,j,n,l} = \sum_{l=1}^{L} S_{n,l}(T_j) f_{v,n,l}(T_j, p_j)$$

where l = 1, ...L in the number of absorbing lines of n-th gas at a selected v; $S_{v,n,l}$ and $f_{v,n,l}$ are the intensity and profile of the l-th line.

Typically, absorption lines within 25 cm⁻¹ of ν are used.

The Lorentz halfwidth is obtained from pressure/temperature scaling:

$$\alpha_i = \alpha_i^0 \left(\frac{p}{p_0}\right) \left(\frac{T_0}{T}\right)^n$$

The foreign and self broadening are added with volume mixing ratio q:

$$\alpha_i^0 = (1 - q)\alpha_{L,air}^0 + q\alpha_{L,self}^0$$

Optical depth $\tau_{\nu,j,n}$, of n-th gas of j-th layer

$$\tau_{v,j,n} = k_{v,n,j} u_{n,j}$$

where $u_{n,j}$ is the slant path for n-gas in j-th layer (i.e., the amount of n-th gas in j-th layer).

Repeating above calculations for all gases n=1, ...N, we find optical depth of j-th layer

$$\tau_{v,j} = \sum_{n=1}^{N} \tau_{v,j,n}$$

Repeating above calculations for all layers j=1, ...J, we find optical depth of each layer.

Using calculated optical depth of each layer, we find the **monochromatic upward and downward intensities** from Eq.[8.3a,b].

NOTE: Similar strategy is used to solve Eq.[4.4a,b] via monochromatic transmission function:

for n-th gas

$$T_{v,j,n} = \exp(-\frac{\tau_{v,j,n}}{\mu})$$

and, using the **multiplication law** of transmittance, we have the transmittance of j-th layer of N absorbing gases

$$T_{v,j} = T_{v,1} T_{v,2} ... T_{v,N}$$

Multiplication law of transmittance states that when several gases absorb, the
monochromatic transmittance is a product of the monochromatic transmittances of
individual gases:

$$T_{v,1,2...N} = T_{v,1}T_{v,2}...T_{v,N}$$

❖ For many practical applications, one needs to know not monochromatic intensity (or flux) but intensity (or flux) averaged over a given wavenumber interval.

Spectral intensity = intensity averaged over a very narrow interval that B_{ν} is almost constant but the interval is large enough to consist of several absorption lines.

Narrow-band intensity= intensity averaged over a narrow band which includes a lot of lines;

Broad-band intensity= intensity averaged over a broad band (e.g., over a whole longwave region)

We can define the **spectral transmission function** for a band of a width Δv as

$$T_{\overline{v}}(u) = \frac{1}{\Delta v} \int_{\Delta v} T_{v}(\tau) dv = \frac{1}{\Delta v} \int_{\Delta v} \exp(-\tau_{v}) dv = \frac{1}{\Delta v} \int_{\Delta v} \exp(-k_{v}u) dv$$

NOTE: **Spectral intensify** requires the calculations of **spectral transmission** which requires the calculations of **monochromatic optical depth** which are done with LBL computations.

Spectral absorptance is defined as

$$A_{\overline{v}} = 1 - T_{\overline{v}}(u) = \frac{1}{\Delta v} \int_{\Delta v} (1 - \exp(-\tau_v)) dv = \frac{1}{\Delta v} \int_{\Delta v} (1 - \exp(-k_v u)) dv$$

[8.6]

LBL spectral resolution:

- Because LBL computes each line of absorbing gases in non-homogeneous atmosphere, the adequate selection of an integration step (i.e., interval dv) is required to calculate the spectral transmittance in the interval Δv ($\Delta v > dv$).
- Because P decreases exponentially with altitude, the line half-width and hence the integration step should be smaller at higher altitudes in the atmosphere.
- Because of these variable resolutions, the absorptions coefficients of two consequent layers must be merged – it is done by interpolating the coarser-resolution of lower layers into the finer-resolution of the higher-level => spectral absorptance for a given slant path is computed with the finest spectral resolution.

Continuum

Absorption lines may have long wings (e.g., depending on a line half-width). To simplify calculations, the wings of a line are cut at a given distance from the line center Thus the absorption coefficient of the line may be expressed as

$$k_{\nu} = Sf_{\nu} + k_{\nu}^{c} \tag{8.7}$$

where k_{ν}^{c} gives the absorption fraction in the wings (called **continuum absorption**).

CKD (Clough, Kneizys, and Davies) continuum model:

includes continuum absorption due to water vapor, nitrogen, oxygen, carbon dioxide, and ozone. The water vapor continuum is based upon a water vapor monomer line shape formalism applied to all spectral regions from the microwave to the shortwave.

The absorption coefficient for the water vapor continuum is the sum of the self- and foreign (air)-broadening components:

$$k_v^c = \sigma_{self} \left[p_w + \frac{\sigma_{air}}{\sigma_{self}} (p - p_w) \right]$$
 [8.8]

where p_w and p denote the water vapor partial pressure and the air (ambient) pressure (in atm), respectively, and σ_{self} and σ_{air} are the self- and air-broadening coefficients for water vapor.

In the 8-12 µm region, the self-broadening coefficient is parameterized as (Roberts et al., 1976):

$$\sigma_{self}(v, T_r) = a + b \exp(-\beta v)$$
 [8.9]

where $T_r = 296 \text{ K}$, a=4.18, b=5578, and b=7.87x10⁻³ (for σ_{self} in cm² g⁻¹ atm⁻¹).

And $\sigma_{air}/\sigma_{self}=0.002$ at $T_r=296$ K.

Moreover, σ_{self} depends on as:

$$\sigma_{self}(v,T) = \sigma_{self}(v,T_r) \exp(c(T_r/T-1))$$

where c=6.08

NOTE: There are two competing effects on absorption of the water vapor continuum: absorption coefficient increases as the temperature decreases, but colder atmospheric conditions have less water vapor.

LBL numerical codes:

LBLRTM is developed in the ATMOSPHERIC AND ENVIRONMENTAL

RESEARCH INC.

http://www.rtweb.aer.com/

FASCODE (FAST Atmospheric Signature CODE)

H.J.P. Smith, D.J. Dube, M.E. Gardner, S.A. Clough, F.X. Kneizys, and L.S. Rothman, FASCODE- Fast Atmospheric Signature Code (Spectral Transmittance and Radiance), Air Force Geophysics Laboratory Technical Report AFGL-TR-78-0081, Hanscom AFB, MA, 1978.

GENLN (General Line-by-Line Atmospheric Transmittance and Radiance Code)

D.P. Edwards.

Genln2: A general line-by-line atmospheric transmittance and radiance model. NCAR Technical Note 367+STR, National Center for Atmospheric Research, Boulder, Colo., 1992.

GENSPECT (General Spectral Toolbox for Radiative Transfer and Gas Spectral

Property Computation, Univ. of Toronto, Canada)

http://www.genspect.com/

1.3. Spectroscopic databases: HITRAN, GEISA, and JPL MS.

HITRAN (HIgh-resolution TRANsmission molecular absorption database)
http://www.hitran.com

The database is a long-running project started by the Air Force Cambridge Research Laboratories (AFCRL) in the late 1960's in response to the need for detailed knowledge of the infrared properties of the atmosphere. The HITRAN compilation, and its analogous database HITEMP (high-temperature spectroscopic absorption parameters), are now being developed at the Atomic and Molecular Physics Division, Harvard-Smithsonian Center for Astrophysics.

The HITRAN'2000 Database (Version 11.0) contains over 1,080,000 spectral lines for 36 different molecules, including the atom O (singlet) and the ion NO⁺.

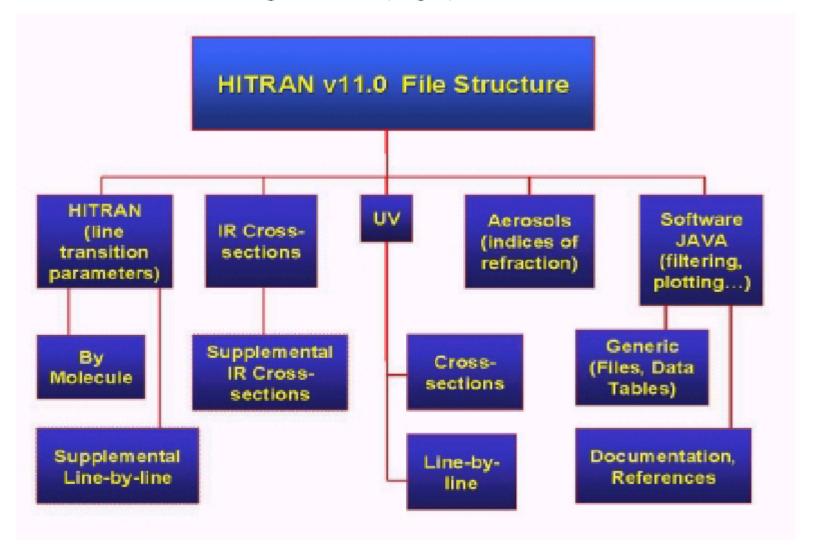


Figure 8.1 The tree structure of the HITRAN2000

GEISA (Gestion et Etude des Informations Spectroscopiques Atmospheriques) http://ara.lmq.polytechnique.fr

GEISA97 contains line parameters for 42 molecules (96 isotopic species) with 1,346,266 entries between 0 and 22,656 cm⁻¹. It has molecules of interest for both terrestrial and other planetary atmospheres (for example, C₂H₄, GeH₄, C₃H₈, C₂N₂, C₄H₂, HC₃N, H₂S, HCOOH and C₃H₄, for the Giant Planets).

JPL MS (Jet Propulsion Laboratory Molecular Spectroscopy)
http://spec.jpl.nasa.gov